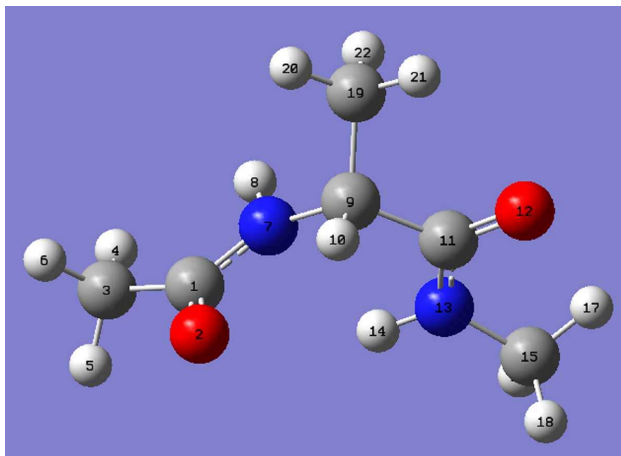


Supplementary Table S1. Comparison of observed bands of polycrystalline powder of N-acetyl-L-alanine-methyl-amide with vibrations calculated by CRYSTAL09. The symmetry of calculated modes is given in Supplementary Material.



observed Raman	observed infrared	calculated CRYSTAL09	mode description
3278 w,br	3257 m	3431,3429,3429,3429	$\nu(\text{NH})$
		3405,3404,3401,3401	$\nu(\text{NH})$
		3388,3386,3371,3371	$\nu(\text{NH})$
		3310,3309,3300,3299	$\nu(\text{NH})$
		3185,3185,3185,3185	$\nu(\text{CH}_3)$
		3179,3179,3179,3179	$\nu(\text{CH}_3)$
		3173,3173,3172,3172	$\nu(\text{CH}_3)$
		3169,3169,3169,3169	$\nu(\text{CH}_3)$
		3161,3161,3161,3161	$\nu(\text{CH}_3)$
		3159,3159,3159,3158	$\nu(\text{CH}_3)$
		3155,3155,3154,3154	$\nu(\text{CH}_3)$
		3144,3144,3143,3143	$\nu(\text{CH}_3)$
		3142,3142,3142,3142	$\nu(\text{CH}_3)$
		3137,3137,3137,3137	$\nu(\text{CH}_3)$
3088 w,br	3081 m	3124,3124,3124,3124	$\nu(\text{CH}_3)$
		3120,3120,3120,3120	$\nu(\text{CH}_3)$
2996 m,sh		3116,3116,3116,3116	$\nu(\text{CH}_3)$
2985 s		3111,3111,3111,3111	$\nu(\text{CH}_3)$
2959 s,sh		3072,3072,3072,3072	$\nu(\text{CH}_3)$
2940 s		3071,3071,3071,3071	$\nu(\text{CH}_3)$
2929 m,sh		3065,3065,3065,3065	$\nu(\text{CH}_3)$
2908 m,sh		3065,3065,3064,3064	$\nu(\text{CH}_3)$
2884 m		3062,3062,3061,3061	$\nu(\text{CH}_3)$
2855 w		3053,3053,3053,3053	$\nu(\text{CH}_3)$

Supplementary Table S1. continued.

observed Raman	observed infrared	calculated CRYSTAL09	mode description
		1735,1731,1731,1726	$\nu(\text{C=O})$
1667 m,sh	1664 s	1724,1723,1722,1721	$\nu(\text{C=O})$
		1717,1716,1705,1697	$\nu(\text{C=O})$
		1696,1692,1686,1686	$\nu(\text{C=O}) + \delta(\text{NH})$
1651 m		1648,1640,1640,1639	$\delta(\text{NH})$
1639 m,sh	1636 vs	1638,1638,1635,1634	$\delta(\text{NH})$
1578 vw ,1567 vw	1553 vs,br	1634,1632,1632,1631	$\delta(\text{NH}) + \nu(\text{C-N})$
1533 vw	1511 s, sh	1625,1623,1621,1619	$\delta(\text{NH}) + \nu(\text{C-N})$
		1537,1536,1535,1534	$\delta(\text{CH}_3)$
		1525,1523,1523,1523	$\delta(\text{CH}_3)$
		1522,1521,1521,1520	$\delta(\text{CH}_3)$
		1519,1519,1519,1518	$\delta(\text{CH}_3)$
		1514,1513,1511,1510	$\delta(\text{CH}_3)$
		1509,1508,1508,1508	$\delta(\text{CH}_3)$
		1506,1505, 1503,1503	$\delta(\text{CH}_3)$
		1503,1503,1502,1502	$\delta(\text{CH}_3)$
		1500,1500,1499,1499	$\delta(\text{CH}_3)$
		1497,1496,1496,1495	$\delta(\text{CH}_3)$
		1495,1495,1489,1489	$\delta(\text{CH}_3)$
		1485,1485,1484,1484	$\delta(\text{CH}_3)$
1460 m,sh	1461 m,sh	1461,1461,1461,1461	$\delta(\text{CH}_3)$
1455 m	1444 m	1452,1451,1451,1451	$\delta(\text{CH}_3)$
1436 mw	1431 m	1434,1434,1433,1433	$\delta(\text{CH}_3)$
		1429,1429,1429,1428	$\delta(\text{CH}_3)$
		1427,1426,1426,1426	$\delta(\text{CH}_3)$
1417 mw		1421,1421,1420,1420	$\delta(\text{CH}_3)$
	1411 m	1411,1411,1411,1410	$\delta(\text{CH}) + \delta(\text{CH}_3)$
		1403,1402,1402,1402	$\delta(\text{CH}) + \delta(\text{CH}_3)$
1386 w		1366,1366,1359,1359	$\delta(\text{NH}) + \delta(\text{CH}_3)$
1379 m	1374 vs	1354,1353,1352,1352	$\delta(\text{NH}) + \delta(\text{CH}_3)$
		1327,1326,1, 326,1326	$\delta(\text{CH})$
1316 mw		1319,1318,1318,1318	$\delta(\text{CH})$
	1311 m	1309,1309,1308,1308	$\delta(\text{NH}) + \delta(\text{CH}_3)$
1287 mw	1281 s	1300,1300,1298,1298	$\delta(\text{NH}) + \delta(\text{CH}_3)$
1262 m	1259 vs	1207,1206,1206,1205	$\nu(\text{C-N})$
		1204,1204,1204,1203	$\nu(\text{C-N})$
		1191,1190,1188,1187	$\delta(\text{CH}_3)$ wagging
1177 m	1178 s	1186,1186,1186,1185	$\delta(\text{CH}_3)$ wagging
1163 m	1160 m,br	1151,1151,1151,1151	$\delta(\text{CH}_3)$ wagging
		1149,1149,1149,1149	$\delta(\text{CH}_3)$ wagging

Supplementary Table S1. continued.

observed Raman	observed infrared	calculated CRYSTAL09	mode description
1131 w		1130,1129,1129,1129	$\nu(\text{C-C})$
1123 w		1121,1121,1121,1120	$\nu(\text{C-C})$
1106 m	1103 w	1088,1088,1088,1088	$\nu(\text{C-N}) + \delta(\text{CH}_3)$
1102 m		1082,1082,1082,1081	$\delta(\text{CH}_3)$
		1073,1073,1072,1072	$\delta(\text{CH}_3)$
		1070,1070,1070,1070	$\delta(\text{CH}_3)$ twisting
1061 mw	1058 m	1060,1060,1060,1060	$\delta(\text{CH}_3)$ rocking
		1052,1052,1052,1051	$\delta(\text{CH}_3)$ rocking
1044 w,sh	1042 m	1038,1038,1038,1037	$\delta(\text{CH}_3)$ twisting
1035 w	1033 m,sh	1037,1036,1035,1035	$\delta(\text{CH}_3)$ rocking
1012 w	1011 m	988,988,986,986	$\nu(\text{C-C})$
964 m	961 m	980,979,979,979	$\nu(\text{C-C})$
		940,940,940,939	$\delta(\text{CH}_3) + \delta(\text{CH})$
917 mw	918 mw	925,924,922,921	$\delta(\text{CH}_3) + \delta(\text{CH})$
		901,900,899,899	$\gamma(\text{NH})$ out of plane
		881,880,879,879	$\delta(\text{CH}_3) + \gamma(\text{NH})$
865 m	864 w	876,875,874,874	$\delta(\text{CH}_3)$
		827,825,821,820	$\gamma(\text{NH})$ out of plane
	806 w,sh	801,800,800,798	$\gamma(\text{NH})$ out of plane
	769 mw	783,783,782,782	$\gamma(\text{NH})$ out of plane
759 vw		746,745,744,744	$\gamma(\text{C-N})$ out of plane
		731,728,725,725	$\gamma(\text{C-N})$ out of plane
	710 m,sh	711,710,710,709	$\delta(\text{N-C-C})$
694 w,br	682 vs,br	703,703,703,703	$\nu(\text{C-N})$
		645,645,643,643	$\delta(\text{O=C-N})$
635 m	634 ms	643,643,642,642	$\delta(\text{O=C-N})$
609 w		622,622,618,618	$\delta(\text{O=C-N})$
597 m	594 vs	609,609,609,608	$\delta(\text{O=C-N})$
		529,528,528,528	$\delta(\text{N-C-C})$
520 m	519 s	525,523,522,522	$\delta(\text{O=C-C}) + \delta(\text{C-C-N})$
		417,417,413,413	$\delta(\text{O=C-N})$
403 m	399 ^l	400,399,397,397	$\delta(\text{O=C-N}) + \delta(\text{C-N-C})$
		384,382,379,378	$\delta(\text{O=C-N}) + \delta(\text{C-N-C})$
369 m	366 ^l	376,374,373,372	$\delta(\text{O=C-N})$
		359,358,357,357	radial column mode
338 m	339 ^l	344,344,344,343	skeletal column mode
		310,309,306,305	$\tau(\text{CH}_3)$
290 m		302,298,298,297	$\tau(\text{CH}_3)$
		271,271,267,266	$\tau(\text{CH}_3)$
253 w		261,259,258,257	$\tau(\text{CH}_3)$

Supplementary Table S1. continued.

observed Raman	observed infrared	calculated CRYSTAL09	mode description
		246,246,244,244	$\tau(\text{CH}_3)$
		241,239,238,238	$\tau(\text{CH}_3)$
		219,217,216,216	$\tau(\text{CH}_3)$
		209,208,205,202	$\tau(\text{CH}_3)$
194 mw		197,197,197,196	$\tau(\text{CH}_3)$
		191,187,187,186	$\tau(\text{CH}_3)$
		179,178,176,175	$\tau(\text{CH}_3)$
		174,170,169,169	$\tau(\text{CH}_3)$
		165,165,158,158	$\tau(\text{CH}_3)$
153 m		157,154,154,152	$\tau(\text{CN})$
		149,149,145,143	$\tau(\text{CN})$
		142,138,135,135	$\tau(\text{CN})$
		130,127,124,122	$\gamma(\text{C=O})$
		120,119,117,116	$\gamma(\text{CN})$
		114,114,113,112	skeletal+lattice
110 ms		109,108,108,105	skeletal+lattice
		105,99,98	skeletal+lattice
96 ms		96,94,93,93	skeletal+lattice
		90,90,89,87	skeletal+lattice
		84,84,82,82	skeletal+lattice
		80,79,77,76	skeletal+lattice
		75,71,71,69	skeletal+lattice
65 s		68,65,64,59	skeletal+lattice
58 s		57,56,54,52	skeletal+lattice
		49,46,45,45	skeletal+lattice
44 vs		45,41,39,37	skeletal+lattice
36 vs		33,32	column deformation
26 vs		26	column deformation
		16	column translation along b

abbreviations: v – stretching, δ – bending, γ -out of plane bending, τ – torsion, vs -very strong, s – strong, ms – medium strong, m – medium, w – weak, sh – shoulder

¹from the ref [24]